Symmetry Operators of Generalized Wreath Products and Their Applications to Chemical Physics

K. BALASUBRAMANIAN*

Department of Chemistry and Lawrence Berkeley Laboratory, University of California, Berkeley, California 94720, U.S.A.

Abstract

Symmetry operators of generalized wreath product groups are formulated. Several applications of these operators to nonrigid molecular problems in chemical physics are outlined.

1. Introduction

In recent years generalized wreath product groups were used as efficient representations of symmetries of molecules exhibiting large amplitude nonrigid motions [1, 2], NMR spin Hamiltonians [3], etc. By the term "large amplitude" we mean amplitudes large in the ordinary experimental NMR scale. Randić [4-7], Balaban [8, 9], and the present author [10] studied the symmetry groups of graphs of chemical interest. The symmetry groups of a number of chemically interesting graphs can be embedded into wreath or generalized wreath products. Balaban and co-workers [11, 12] and Randić [7] have recognized the use of wreath products in such chemical applications. Several other representations of symmetry groups of nonrigid molecules have been developed by other authors [13-20].

The generalized wreath product groups have special structures that provide for elegant derivation of physically interesting quantities. The generalized character cycle indices (GCCI's) of these groups can be obtained in terms of the composing groups. These GCCI's are the generators of spin species, NMR spin multiplets and nuclear spin statistical weights. The nuclear spin statistical weights of the rovibronic levels are of fundamental importance in molecular spectroscopy. They provide information on the intensities of allowed inter-rovibronic transitions. Thus the combinational numbers generated from the GCCI's are prints of the intensity ratios of the various peaks appearing in a molecular spectra.

In this paper we will first briefly outline the preliminary combinatorial concepts. In Section 3 formalisms related to the symmetry operators of generalized wreath products are outlined. In Section 4 applications to the symmetry groups of nonrigid molecules is considered. Section 5 concludes with generalized isomer enumerations. For several chemical applications of graph theory the readers are referred to the book by Balaban [21] and related papers by Randić [22-28], Balaban [29-33], the present author [34-42], and Dolhaine [43].

* Part of the work presented here was done at The Johns Hopkins University, Baltimore, MD 21218.
2. Preliminaries

Let $D$ and $R$ be finite sets and let $|D|$ and $|R|$ denote the number of elements in $D$ and $R$, respectively. Let $G$ be a permutation group acting on $D$. Consider the set of maps from $D$ to $R$. Let $R^D$ denote the set of all such maps. In several situations we may need to consider maps from the cartesian product $A \times B$ ($A$ and $B$ being two finite sets) to $R$ or from the union of several such cartesian products to $R$. The permutation group $G$ acting on $D$ induces permutations on $F = R^D$ by the following recipe:

$$gf(i) = f(g^{-1}i) \quad \text{for } i \in D; f \in R^D.$$ 

Let $V$ be a vector space over a field $K$ of characteristic zero [44] with $\dim V = |R| = r$, and let $e_1, e_2, \ldots, e_r$ be a standard basis of $V$. With each $f \in R^D$, we can associate the tensor product $e_f = e_{f(1)} \otimes e_{f(2)} \otimes \cdots \otimes e_{f(d)}$ and the set of such tensors forms the basis of the $d$th tensor product of $V$. For $g \in G$, we define the permutation operator $P(g)$ with respect to this basis set by $P(g) e_f = e_{gf} = e_{gf(1)} \otimes e_{gf(2)} \otimes \cdots \otimes e_{gf(d)} = e_{f(g^{-1}1)} \otimes e_{f(g^{-1}2)} \otimes \cdots \otimes e_{f(g^{-1}d)}$. Let $\omega : G \to K$ be a nonzero homomorphism [i.e., $\omega(g_1 g_2) = \omega(g_1) \omega(g_2)$, a character of degree 1]. We define a symmetry operator $T_G$ as

$$T_G = \frac{1}{|G|} \sum_{g \in G} \omega(g) P(g).$$

Consider a map $W$ from $F$ to $K$, $W : F \to K$, which is also a constant on the orbits resulting from the action of $G$ on $F$. If $W$ also satisfies the following property for every $f$, it is referred to as a weight function:

$$W(f) = \prod_{i=1}^{d} w(f(i)),$$

where $w$ is a function, $w : R \to K$. $W(f)$ is also referred to as a weight of a function in combinatorics book [45].

Consider the subspace $V_x^d$ of $V^d$ (where $V^d$ is the $d$th tensor product of $V$) spanned by all tensors $S_x = \{e_f : W(f) = x \in K\}$. Let the restrictions of the operators $T_G$ and $P(g)$ to the space $V_x^d$ be $T_G^x$ and $P_x(g)$, respectively. Now define the weighted permutation operator $P_w(g)$ and the weighted symmetry operator $T_G^w$ with the weight $W$ as

$$P_w(g) = \bigoplus_{x \in K} x P_x(g),$$

$$T_G^w = \bigoplus_{x \in K} x T_G^x,$$

where $\oplus$ denotes a direct sum. (See Ref. 46 for a definition of direct sum.) If one considers a matrix representation of $P_w(g)$, then we have

$$\text{Tr} P_w(g) = \sum_{f} W(f),$$
where the sum is taken over all \( f \) for which \( gf = f \). Williamson [47] proved the following theorem. (See also Merris [47].)

**Theorem 1**

\[
T^W_G = \frac{1}{|G|} \sum_{g \in G} \omega(g) P_W(g).
\]

Thus

\[
\text{Tr} \ T^W_G = \frac{1}{|G|} \sum_{g \in G} \omega(g) \text{Tr} [P_W(g)] = \frac{1}{|G|} \sum_{g \in G} \omega(g) \sum_f W(f).
\]

If one defines the generalized character cycle index (GCCCI) of a group \( G \) with character \( \chi \) corresponding to the irreducible representation \( \Gamma \), as

\[
P^\chi_G(s_1, s_2, \ldots) = \frac{1}{|G|} \sum_{g \in G} \chi(g) s_1^{b_1} s_2^{b_2} \cdots,
\]

where \( s_1^{b_1} s_2^{b_2} \cdots \) is a representation of a typical permutation \( g \in G \) having \( b_1 \) cycles of length 1, \( b_2 \) cycles of length 2, etc. Then by Theorem 1 and the preliminary combinatorial results in Ref. 45, we get

\[
\text{Tr} \ T^W_G = P^\chi_G \left( \sum_{r \in R} w(r), \sum_{r \in R} [w(r)]^2, \ldots \right).
\]

A special case of this result for the totally symmetric representation is Pólya's theorem [48].

We now proceed to the symmetry operators of generalized wreath products.

### 3. Symmetry Operators of Generalized Wreath Product Groups

Let a set \( \Omega = \{1, 2, \ldots, n\} \) be partitioned into the mutually disjoint sets \( Y_1, Y_2, \ldots, Y_t \). Let \( G \) be a permutation group acting on \( \Omega \) such that all its orbits are within the same \( Y \) sets. Let \( H_1, H_2, \ldots, H_t \) be \( t \) permutation groups and let \( \Pi_i \) be a map from \( Y_i \) to \( H_i \) (for \( i = 1, 2, \ldots, t \)). Then the set \( \{(g; \Pi_1, \Pi_2, \ldots, \Pi_t) | g \in G, \Pi_i : Y_i \to H_i \} \) is called a generalized wreath product and is denoted as \( G[H_1, H_2, \ldots, H_t] \). Let \( G_i \) be the set of all cycle products contained in the set \( Y_i \). It is shown in Ref. 1 that \( G_i \) forms a group. The multiplication of the elements of generalized wreath product is defined as follows:

\[
(g; \Pi_1, \Pi_2, \ldots, \Pi_t) \cdot (g'; \Pi'_1, \Pi'_2, \ldots, \Pi'_t) = (gg'; \Pi_1 \Pi'_1 \Pi_2 \Pi'_2 \ldots, \Pi_t \Pi'_t),
\]

with

\[
\Pi'_t(j) = \Pi'_t(g_i^{-1} j),
\]
where $g_i$ is the cycle product of $g$ contained in $Y_i$. The product $(H_1^{m_1} \times H_2^{m_2} \times \cdots \times H_t^{m_t}) \cdot G'$ is a permutation representation of $G[H_1, H_2, \ldots, H_t]$, where $H_i^{m_i} = H_1 \times H_2 \times \cdots \times H_{im_i}$.

$G' = \{ (g; e_1, e_2, \ldots, e_t) | g \in G, e_i(j) = 1 \}$ (the identity of group $H_i$) $\forall j \in Y_i$, and $H_{ij}$ is a copy of the group $H_i$. The special case of this group with $t = 1$ is the well-known wreath product denoted as $G[H]$.

Let the irreducible representations of $H_1^{m_1} \times H_2^{m_2} \times \cdots \times H_t^{m_t}$ be denoted $F_1^{m_1} \times F_2^{m_2} \times \cdots \times F_t^{m_t}$, where $F_i^{m_i}$ is the outer tensor product $F_{i1} \times F_{i2} \times \cdots \times F_{im_i}$, with $F_{ij}$ being an irreducible representation of $H_i$. The group $G$ acts on the set of $\#_i F_i^{m_i}$'s and partitions them into equivalence classes. The inertia group of each such class should be determined where the inertia group consists of the set of those permutations satisfying the following property:

$$G[\{H_1, H_2, \ldots, H_t\}] = \{ (g; \Pi_1, \Pi_2, \ldots, \Pi_t) | \Gamma(g; \Pi_1, \Pi_2, \ldots, \Pi_t) = \Gamma \}$$

where

$$\Gamma = \#_i F_i^{m_i},$$

with

$$F^* (g; \Pi_1, \Pi_2, \ldots, \Pi_t) = F^* (g; \Pi_1, \Pi_2, \ldots, \Pi_t)^{-1} \times (\pi_1, \pi_2, \ldots, \pi_t) (g; \Pi_1, \Pi_2, \ldots, \Pi_t).$$

A permutation representation of the inertia group $G[\{H_1, H_2, \ldots, H_t\}]$ is $(H_1^{m_1} \times H_2^{m_2} \times \cdots \times H_t^{m_t}) \cdot G'$, where $G'$ is known as the inertia factor. If one knows the representation matrices of $(F_1^{m_1} \times F_2^{m_2} \times \cdots \times F_t^{m_t}) (e; \pi_1, \pi_2, \ldots, \pi_t)$ it is possible to find the representation matrices of $(F_1^{m_1} \times F_2^{m_2} \times \cdots \times F_t^{m_t}) (g; \pi_1, \pi_2, \ldots, \pi_t)$ by a suitable permutation of the columns of $\#_i F_i^{m_i}$ determined by $g^{-1}$ as described in Ref. 1. The group $G$ acting on $\Omega$ must be intransitive. This is implicit in partitioning the set $\Omega$ into disjoint sets $Y_1, Y_2, \ldots, Y_t$ and stipulating that every $g \in G$ has all its orbits within the same $Y_i$ sets. Let $T_1, T_2, \ldots, T_t$ be $t$ sets. $T$'s are usually referred to as types. Then the generalized wreath product $G[H_1, H_2, \ldots, H_t]$ with $H_i$ acting on $T_i$ acts on $\cup_{i=1}^t Y_i \times T_i$. A typical $(g; \Pi_1, \Pi_2, \ldots, \Pi_t) \in G[H_1, H_2, \ldots, H_t]$ acts on $\cup_{i=1}^t Y_i \times T_i$ as follows:

$$(g; \Pi_1, \Pi_2, \ldots, \Pi_t) (y; t) = (gy; \Pi_i(y)t) \quad \text{if } y \in Y_i \quad \text{and} \quad t \in T_i.$$ 

Consider the set of maps from $\cup_{i=1}^t Y_i \times T_i$ to a set $R$ and let such a set of maps be denoted

$$R^{\cup_{i=1}^t Y_i \times T_i}.$$ 

The action of $G[H_1, H_2, \ldots, H_t]$ on $\cup_{i=1}^t Y_i \times T_t$ in turn, induces permutations on $R^{\cup_{i=1}^t Y_i \times T_t}$, for a $(g; \Pi_1, \Pi_2, \ldots, \Pi_t) \in G[H_1, H_2, \ldots, H_t]$ and $f \in R^{\cup_{i=1}^t Y_i \times T_t}$:

$$(g; \Pi_1, \Pi_2, \ldots, \Pi_t) f (y, t) = \Pi_i (g^{-1} y) f (g^{-1} y, t) \quad \text{if } y \in Y_i \quad \text{and} \quad t \in T_i.$$
Let \( W : R^{|Y_i|} \times Y_i \to K \) be defined by
\[
W(f) = \prod_{(y, t) \in Y_i \times T_i} w(f(y, t)),
\]
where \( w : R \to K \). \( W \) is a weight function which is also a constant on the orbits of \( G[H_1, H_2, \ldots, H_t] \).

Let \( \lambda_i : H_i \to K \), \( \chi : G \to K \) be characters of degree 1. For a \( \Pi_i \in H_i^{Y_i} \) define
\[
\lambda_i(\Pi_i) = \prod_{y \in Y_i} \lambda_i(\Pi_i(y)).
\]
This is just a \(|Y_i|\)-fold repeated product of \( \lambda_i \). Let \( \omega(g; \Pi_1, \Pi_2, \ldots, \Pi_t) \) be defined by
\[
\omega(g; \Pi_1, \Pi_2, \ldots, \Pi_t) = \chi(g) \lambda_1(\Pi_1) \lambda_2(\Pi_2) \cdots \lambda_t(\Pi_t).
\]
Then note that \( \omega(g; \Pi_1, \Pi_2, \ldots, \Pi_t) \) is a character of \( G[H_1, H_2, \ldots, H_t] \) with degree 1.

Let \( V \) be a vector space over the field \( K \) with \( \dim V = |R| \). Define symmetry operator \( T_{H_i} \), whose range space is \( \otimes Y_i | V \), as
\[
T_{H_i} = \frac{1}{|H_i|} \sum_{h \in H_i} \lambda_i(h) P(h).
\]

Let the vector space spanned by the basis \( \{ e_{f_i} : f_i \in \Delta_{Y_i} \} \) be denoted as \( V_{H_i}^{\Delta_{Y_i}} \):
\[
\Delta_{H_i} = \left\{ y \in R^D \mid \sum_{\sigma \in H_i(y)} \lambda_i(\sigma) \neq 0 \right\}.
\]

Then the symmetry operator of \( G \) can be defined over the tensor product space
\[
\otimes V_{H_1}^{\Delta_{Y_1}} \otimes V_{H_2}^{\Delta_{Y_2}} \otimes \cdots \otimes V_{H_t}^{\Delta_{Y_t}}
\]
by
\[
T_G = \frac{1}{|G|} \sum_{g \in G} \chi(g) P(g).
\]

With \( \omega \) defined as above the symmetry operator \( T_{G[H_1, H_2, \ldots, H_t]} \) can be defined as
\[
T_{G[H_1, H_2, \ldots, H_t]} = \frac{1}{|G[H_1, H_2, \ldots, H_t]|} \sum_{g \in G} \omega(g; \Pi_1, \Pi_2, \ldots, \Pi_t) P(g; \Pi_1, \Pi_2, \ldots, \Pi_t).
\]

In this setup one can generalize Williamson’s theorem [50] to Theorem 2 stated below for Abelian characters.

**Theorem 2**

The weighted symmetry operators
\[
T_{G[H_1, H_2, \ldots, H_t]}^\omega, \ T_{G[H_1, H_2, \ldots, H_t]}^T, \ T_{H_1}^{H_2 Y_1}, T_{H_2^{H_2 Y_2}}, \ldots, T_{H_t^{H_t Y_t}}
\]
are related as follows:
\[
T_{G[H_1, H_2, \ldots, H_t]}^\omega = T_{G[H_1, H_2, \ldots, H_t]}^\omega T_{H_1^{H_2 Y_1}} T_{H_2^{H_2 Y_2}} \cdots T_{H_t^{H_t Y_t}},
\]
where \( T_{H_i^{Y_i}} \) is the symmetry operator which corresponds to the group \( H_i^{Y_i} \).

If now one follows Williamson’s method [50] of taking traces, it can be shown that
\[
\text{Tr} T_{G[H_1, H_2, \ldots, H_t]}^{\omega} = P_{G[H_1, H_2, \ldots, H_t]}^\omega \left( s_k \to \sum_{r \in R} w^k(r) \right),
\]
where \( P_{G[H_1, H_2, \ldots, H_t]}^\omega \) is obtained as follows:
where $C_{ij}(g)$ is the number of $j$ cycles of $g$ in the set $Y_i$. Let $Z_{ij}^\lambda = Z_i^\lambda (s_k \rightarrow s_{kj})$, where the subscript on the $s$ variables are products. Then

$$P_G^\omega = P_G(s_{ij} \rightarrow Z_{ij}^\lambda).$$

Let us illustrate Theorem 2 with a simple example from NMR groups, namely, the NMR group of propane, $S_2[S_3, S_2]$. Consider the irreducible representation $([3] \# [3]) \# [2] \otimes [1^2]$ of $S_2[S_3, S_2]$. This is an one-dimensional representation:

$$P_G^{[1^2]} = \frac{1}{2}(s_1 s_{21} - s_{21} s_2),$$

$$Z_{11} = \frac{1}{2}(s_1^3 + 2s_3 + 3s_1 s_2),$$

$$Z_{12} = \frac{1}{2}(s_3^2 + 2s_6 + 3s_2 s_4),$$

$$Z_{21} = \frac{1}{2}(s_1^2 + s_2),$$

$$P_G^\omega (s_{ij} \rightarrow Z_{ij})$$

$$= \frac{1}{144} [3(s_1^3 + 2s_3 + 3s_1 s_2)^2 \cdot \frac{1}{2}(s_1^3 + s_2) - \frac{1}{6}(s_2^3 + 2s_6 + 3s_2 s_4) \cdot \frac{1}{2}(s_1^2 + s_2)]$$

$$= \frac{1}{144}(s_1^8 + 4s_1^3 s_2^2 + 15s_1^2 s_2^4 + 4s_1 s_2^3 + 16s_1^3 s_2 s_3 + 7s_1^6 s_2 + 4s_2 s_3^3 + 3s_1^2 s_2)$$

$$+ 12s_1 s_2^3 s_3 - 12s_1^2 s_6 - 18s_1^2 s_2 s_4 - 6s_2^4 - 12s_2 s_6 - 18s_2^2 s_4).$$

Thus, $Tr_{G_{[H_1, H_2, \ldots, H_t]}}$ with $\Gamma: ([3] \# [3]) \# [2] \otimes [1^2]$ is

$$\frac{1}{144} \left[ \left( \sum_{r \in R} w(r) \right)^8 + 4 \left( \sum_{r \in R} w(r) \right)^2 \left( \sum_{r \in R} w^3(r) \right)^2 \right]$$

$$+ 15 \left( \sum_{r \in R} w(r) \right)^4 \left( \sum_{r \in R} w^2(r) \right)^2 + 4 \left( \sum_{r \in R} w(r) \right)^5$$

$$\times \left( \sum_{r \in R} w^3(r) \right) + 12 \left( \sum_{r \in R} w(r) \right)^3 \left( \sum_{r \in R} w^2(r) \right)$$

$$\times \left( \sum_{r \in R} w^3(r) \right) + 7 \left( \sum_{r \in R} w(r) \right)^6 \left( \sum_{r \in R} w^2(r) \right)$$

$$+ 4 \left( \sum_{r \in R} w^2(r) \right) \left( \sum_{r \in R} w^3(r) \right)^2 + 3 \left( \sum_{r \in R} w(r) \right)^2$$
Let the inertia group of a representation $F^* = F_1^* \circ F_2^* \circ \cdots \circ F_t^*$ be $G_{F^*}[H_1, H_2, \ldots, H_t]$ and let $G_{F^*}$ be the corresponding inertia factor. Then we have the following generalization for non-Abelian characters:

Define $P_{GF^*}$ to be

$$P_{GF^*} = \frac{1}{|G_{F^*}|} \sum_{g \in G_{F^*}} \prod_{i, j} \chi(g)s_{ij}^{C_{ij}(g)},$$

where $C_{ij}(g)$ denotes the number of $j$ cycles of $g$ in the set $Y_i$, where $Y_i$ is defined as in Section 3, and $\chi$ is the character of the representation $F$ of the group $G_{F^*}$ equivalent to $F'$ of $G_{F^*}$ appearing in the representation

$$\Gamma = (F_1^* \circ F_2^* \circ \cdots \circ F_t^*) \otimes F' \uparrow G[H_1, H_2, \ldots, H_t].$$

Let $Z_{j}^{\lambda_k}$ be defined as discussed above, but now $\lambda_k$ is defined by the representations appearing in the outer tensor product $F_t^*$. Then

$$P_{F^*}(G[H_1, H_2, \ldots, H_t]) = P_{GF^*}(s_{ij} \rightarrow Z_{j}^{\lambda_k})$$

if this $j$ cycle in $Y_i$ is constituted by $j$ copies of the representation whose character is $\lambda_k$. The corresponding generating function is obtained by the following substitution:

$$G \cdot F = P_{F^*}(G[H_1, H_2, \ldots, H_t]) \left( s_k \rightarrow \sum_{r \in R} w^k(r) \right).$$

Let us illustrate the above procedure with two examples of non-Abelian characters from the group $S_2[S_3, S_2]$.

Let $\Gamma$ be $[2, 1] \neq [2, 1] \neq [1^2]^\uparrow \uparrow S_2[S_3, S_2]$. The inertia group of $[2, 1] \neq [2, 1] \neq [1^2]$ is $S_2[S_3, S_2]$. The cycle index of the group $S_2$ isomorphic to the inertia factor with the character which corresponds to the irreducible representa-
tion \([1^2]\) is

\[
P_{S_2}^{[1^2]} = \frac{1}{6}(s_{11}s_{21} - s_{21}s_{12}),
\]

\[
Z_{11}^{[1^2]} = \frac{1}{3}(s_{2}^3 - s_{2}),
\]

\[
Z_{12}^{[1^2]} = \frac{1}{3}(s_{3}^2 - s_{6}),
\]

\[
Z_{21}^{[1^2]} = \frac{1}{2}(s_{1}^2 - s_{2}).
\]

Thus,

\[
P_{(S_2[S_3, S_2])} = \frac{1}{6}[\left( s_{1}^3 - s_{3} \right)^2 \cdot \frac{1}{2} \cdot (s_{1}^2 - s_{2}) - \frac{1}{3}(s_{1}^2 - s_{2}) \cdot \frac{1}{2} \cdot (s_{2}^3 - s_{6})]
\]

\[
= \frac{1}{144}[4s_{1}^8 - 8s_{1}s_{3} + 4s_{1}s_{2}^2 - 4s_{6}s_{2} + 8s_{3}s_{3}s_{3} - 4s_{3}s_{3}^2
\]

\[-12s_{2}^2s_{2}^3 + 12s_{4}^2 + 12s_{7}s_{6} - 12s_{2}s_{6}].
\]

Let \(\Gamma\) be \([1^3]\# [2, 1] \# [2] \otimes [1]\# S_2[S_3, S_2].\) For this case the inertia group is \(S_3 \times S_3 \times S_2,\) and hence the inertia factor is the trivial group containing only the identity. In fact, \(\Gamma\) is equivalent to \([1^3]\# [2, 1] \# [2]\# S_2[S_3, S_2]:\)

\[
P_{S_1}^{[1]} = s_{11}s_{21} \quad \text{(corresponds to (1)(3)(2)),}
\]

\[
Z_{11}^{[1]} = \frac{1}{6}(s_{1}^3 + 2s_{3} - 3s_{1}s_{2}),
\]

\[
Z_{12}^{[1]} = \frac{1}{3}(s_{2}^3 - s_{3}),
\]

\[
Z_{21}^{[1]} = \frac{1}{2}(s_{1}^2 + s_{2}),
\]

\[
P_{S_2[S_3, S_2]}^{[1]} = \frac{1}{6}(s_{1}^3 + 2s_{3} - 3s_{1}s_{2}) \cdot \frac{1}{3} \cdot (s_{3}^3 - s_{3}) \cdot \frac{1}{2}(s_{1}^2 + s_{2}).
\]

(The first factor in the product \(s_{11}s_{11}\) is a consequence of the first representation in the outer product \([1^3]\# [2, 1],\) while the second is a result of \([2, 1].\) Hence we have the above substitution.) The corresponding generating functions can be readily obtained for both the representations.

4. Applications to Nonrigid Molecules

The GCCI's of generalized wreath products can thus be obtained in terms of the GCCI's of the composing groups. Consequently, characters of all the classes with the same cycle type of the generalized wreath product can be generated from character tables of groups of much lower order. This has an important application in obtaining the character tables of the symmetry groups of nonrigid molecules which are, in general, generalized wreath product groups \([1].\) Note that the coefficient of \(x_{1}^{a_1}x_{2}^{b_2} \cdots \) (\(x\)'s are dummy symbols like \(s'\)) in \(P_{G_{\infty}}^{\Gamma}\), which can be obtained in terms of \(P_{G_{\infty}}^{\Gamma}\) and \(Z_{a}^{x_{i}}s_{i}'\) gives the sum of characters of elements of \(G[H_1, H_2, \ldots, H_i]\) with the same cycle type. Since all the elements in the same conjugacy class have the same cycle type the coefficient of \(x_{1}^{a_1}x_{2}^{b_2} \cdots \) gives

\[
\sum_{C} \chi(C)|C|,
\]
where the sum is taken over all $C$ with the same cycle type $x_1^{l_1}x_2^{l_2} \cdots$. $\chi(C)$ is the character $\chi$ in the conjugacy class $C$ and $|C|$ is the order of the conjugacy class $C$. When there is only one conjugacy class with the same cycle type $x_1^{l_1}x_2^{l_2} \cdots$ (which is very often the case) the coefficient of $x_1^{l_1}x_2^{l_2} \cdots$ gives $\chi(C)|C|$ and thus the character $\chi(C)$ is generated. When there are more than one conjugacy classes with the same cycle type, if we determine the characters of all but one conjugacy class with the methods outlined in Ref. 1, using the coefficient of $x_1^{l_1}x_2^{l_2} \cdots$ in $P^T(G[H_1,H_2,\ldots,H_t])$ the character of the last conjugacy class can be determined. In practice, for several wreath products and generalized wreath products, at most two or three conjugacy classes have the same cycle type and several conjugacy classes have the unique cycle type. Thus $P^T(G[H_1,H_2,\ldots,H_t])$, which is obtained very elegantly and easily provides for inventories of characters of all the irreducible representations of wreath and generalized wreath products.

We now illustrate this method with examples. We give two examples, namely, $C_2[C_3]$ and $S_2[S_4]$, where there is no 1-1 correspondence between cycle representation and conjugacy classes. In Table I, the character table of the cyclic group $C_3$ is shown with $\gamma_1$ and $\gamma_2$ treated as components of the degenerate representation $E$. Table II shows the various GCCI’s of group $C_3$. The two GCCI’s of group $C_2$ are readily obtained. The irreducible representations of $C_2[C_3]$ and their GCCI’s are shown in Table III. They were obtained in terms of the GCCI’s of $C_3$ shown in Table II and those of $C_2$. For example, the GCCI $P^{12}$ for $\Gamma_2 = (A_1 \neq A_1) \otimes [1^2]$ is given by the following substitutions:

\[
p^{[12]} = \frac{1}{2}(x_1^2 - x_2) \quad \text{(there is only one Y set)},
\]

\[
Z_{11}^{A_1} = \frac{1}{3}(x_1^3 + 2x_3) \quad \text{(from Table II)},
\]

\[
Z_{12}^{A_1} = \frac{1}{3}(x_2^2 + 2x_6).
\]
TABLE II. GCCI's of the cyclic group $C_3$. Note that the sum of the GCCI's of $\gamma_1$ and $\gamma_2$ is the GCCI of $E$.

<table>
<thead>
<tr>
<th>$\Gamma$</th>
<th>$3\Phi_\Gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1$</td>
<td>$x_1^3 + 2x_3$</td>
</tr>
<tr>
<td>$\gamma_1$</td>
<td>$x_1^3 + (\omega + \omega^*) x_3$</td>
</tr>
<tr>
<td>$\gamma_2$</td>
<td>$x_1^3 + (\omega^* + \omega) x_3$</td>
</tr>
<tr>
<td>$E$</td>
<td>$2x_1^3 - 2x_3$</td>
</tr>
</tbody>
</table>

Thus, we have

$$P_2^\Gamma = p^{[12]}(x_{ij} \rightarrow Z_{ij}^h)$$

$$= \frac{1}{12}(x_1^3 + 2x_3)^2 - \frac{1}{3}(x_2^3 + 2x_6))$$

$$= \frac{1}{18}(x_1^6 + 4x_1^3x_3 + 4x_3^2 - 3x_2^3 - 6x_6).$$

TABLE III. GCCI's of $C_2[C_3]$ obtained using the procedure outlined in this paper from the GCCI's of $C_2$ and $C_3$.

<table>
<thead>
<tr>
<th>No.</th>
<th>$\Gamma$</th>
<th>$18 \Phi_\Gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>$(A_1 # A_1) \otimes [2]'$</td>
<td>$x_1^6 + 4x_1^3x_3 + 4x_2^3 + 3x_2^3 + 6x_6$</td>
</tr>
<tr>
<td>2.</td>
<td>$(A_1 # A_1) \otimes [12]'$</td>
<td>$x_1^6 + 4x_1^3x_3 + 4x_2^3 - 3x_2^3 - 6x_6$</td>
</tr>
<tr>
<td>3.</td>
<td>$\left{(\gamma_1 # \gamma_1) \otimes [2]' \right}$</td>
<td>$x_1^6 + (\omega+\omega^<em>)^2 x_3^2 + 2(\omega+\omega^</em>)x_1^3x_3 + 3x_2^3 + 3(\omega+\omega^*)x_6$</td>
</tr>
<tr>
<td></td>
<td>$\left{(\gamma_2 # \gamma_2) \otimes [3]' \right}$</td>
<td>$x_1^6 + (\omega^<em>+\omega)^2 x_3^2 + 2(\omega^</em>+\omega)x_1^3x_3 + 3x_2^3 + 3(\omega^*+\omega)x_6$</td>
</tr>
<tr>
<td>4.</td>
<td>$\left{(\gamma_1 # \gamma_2) \otimes [2]' \right}$</td>
<td>$x_1^6 + (\omega+\omega^<em>)^2 x_3^2 + 2(\omega+\omega^</em>)x_1^3x_3 - 3x_2^3 - 3(\omega+\omega^*)x_6$</td>
</tr>
<tr>
<td></td>
<td>$\left{(\gamma_2 # \gamma_2) \otimes [3]' \right}$</td>
<td>$x_1^6 + (\omega^<em>+\omega)^2 x_3^2 + 2(\omega^</em>+\omega)x_1^3x_3 - 3x_2^3 - 3(\omega^*+\omega)x_6$</td>
</tr>
<tr>
<td>5.</td>
<td>$(\gamma_1 # \gamma_2) \otimes C_2[C_3]$</td>
<td>$2x_1^6 - 4x_1^3x_3 + 2x_3^2$</td>
</tr>
<tr>
<td>6.</td>
<td>$(A_1 # E) \otimes C_2[C_3]$</td>
<td>$4x_1^6 + 4x_1^3x_3 - 8x_3^2$</td>
</tr>
</tbody>
</table>

OR

$$\left\{\begin{array}{l}
2x_1^6 - 2(\omega+\omega^*)x_1^3x_3 - 2x_3^2 + 2(\omega+\omega^*)x_3^2 \\
2x_1^6 - 2(\omega^*+\omega)x_1^3x_3 - 2x_3^2 + 2(\omega^*+\omega)x_3^2
\end{array}\right.$$. 
There are two conjugacy classes with the cycle type $x_1^3x_3$, three conjugacy classes with the cycle type $x_2^3$, two conjugacy classes with the cycle type $x_6$, and all other cycle types have unique conjugacy classes. Thus, if the character of the conjugacy class $(123)$ in $\Gamma_2$ is determined by the method in Ref. 1 to be 1, then the character of the conjugacy class $(132)$ is determined as 1 using the gcci, since the coefficient of $x_1^3x_3$ is +4 in $18P^{1,2}$. The characters of $E$ and $(14)(25)(36)$ are immediately determined using gcci’s. The character table thus obtained is shown in Table IV.

The complete character table of the $PI$ group can be obtained by including the inversion operations as a semidirect product. Another nontrivial example is the group $S_2[S_4]$. The character table of $S_4$ and the gcci’s of $S_4$ are shown in Tables V and VI, respectively. Table VII shows the gcci’s of the 20 irreducible representations of $S_2[S_4]$ obtained using the method developed in this paper. The group $S_2[S_4]$ has two conjugacy classes with the cycle type $x_1^4x_2^2$, two classes with the cycle type $x_1^2$, two classes with the cycle type $x_2^3x_4$, and two with the cycle type $x_2^4$. The rest of the 12 conjugacy classes have unique cycle types. Thus $P\Gamma$’s of $S_2[S_4]$ generate the characters of these 12 conjugacy classes immediately, while the characters of other conjugacy classes are determined using $P\Gamma$ and by knowing the character of one of the conjugacy classes with the method in Ref. 1. The character table thus obtained is shown in Table VIII. The conjugacy classes, order of each conjugacy class and the representatives of each conjugacy class.
are obtained using the method in Ref. 1. Table VIII is in agreement with the compound character table, \([8]+[62]+[4^2]\) in Ref. 49. \(C_2[C_3]\) is the rotational subgroup of nonrigid ethane. The fact that \(S_2[S_4]\) is the NMR group of bicyclobutadienyl sandwich complex can be seen using the diagrammatic technique for the characterization of the NMR group of molecules presented in Ref. 3. The permutation representation of the conjugacy classes were obtained using the permutation representation of the wreath product groups outlined in Section 2 and Ref. 1.

As a last example to illustrate how the GCCI's of wreath products can be obtained, consider the third GCCI in Table VII. The irreducible representation under consideration is \([4] \neq [31] S_2[S_4]\). The inertia factor of \([4] \neq [31]\) is \(S_1\), the group containing just \((1)(2)\). The cycle index corresponding to the only identity representation \([2]\) of this group is

\[ p^{[2]} = x_{11}^2. \]

<table>
<thead>
<tr>
<th>(r)</th>
<th>(24\ p^r)</th>
</tr>
</thead>
<tbody>
<tr>
<td>([4])</td>
<td>(x_1^4 + 6x_1^2 x_2 + 8x_1 x_3 + 6x_4 + 3x_2^2)</td>
</tr>
<tr>
<td>([1^4])</td>
<td>(x_1^4 - 6x_1^2 x_2 + 8x_1 x_3 - 6x_4 + 3x_2^2)</td>
</tr>
<tr>
<td>([31])</td>
<td>(3x_1^4 + 6x_1^2 x_2 - 6x_4 - 3x_2^2)</td>
</tr>
<tr>
<td>([21^2])</td>
<td>(3x_1^4 - 6x_1^2 x_2 + 6x_4 - 3x_2^2)</td>
</tr>
<tr>
<td>([2^2])</td>
<td>(2x_1^4 - 8x_1 x_3 + 2x_2^2)</td>
</tr>
<tr>
<td>( \Gamma )</td>
<td>( 1152 , \Gamma )</td>
</tr>
<tr>
<td>---</td>
<td>---</td>
</tr>
</tbody>
</table>
| \([4][43] \otimes [2]^{12} \) | \( \begin{align*} x_1^8 &+ 12x_1^6 x_2 + 16x_1^5 x_3 + 12x_1^4 x_4 + 42x_1^4 x_2 x_3 + 36x_1^2 x_2^3 \\
+ 96x_1^3 x_2 x_3 + 72x_1^2 x_2^2 x_4 + 64x_1^2 x_2 x_3^2 + 48x_1 x_3 x_4 &+ 96x_1 x_3 x_4 \\
+ 144x_8 &+ 108x_4^2 + 180x_2^2 x_4 + 192x_2^2 x_6 + 36x_6^2 \end{align*} \) |
| \([4][43] \otimes [12]^{12} \) | \( \begin{align*} x_1^8 &+ 12x_1^6 x_2 + 16x_1^5 x_3 + 12x_1^4 x_4 + 42x_1^4 x_2 x_3 + 36x_1^2 x_2^3 \\
+ 96x_1^3 x_2 x_3 + 72x_1^2 x_2^2 x_4 + 64x_1^2 x_2 x_3^2 + 48x_1 x_3 x_4 &+ 96x_1 x_3 x_4 \\
- 144x_8 &- 36x_4^2 - 108x_2^2 x_4 - 192x_2^2 x_6 - 15x_6^2 \end{align*} \) |
| \([4][31] \otimes [S_2 [S_4]] \) | \( \begin{align*} 6x_1^8 &+ 48x_1^6 x_2 + 48x_1^5 x_3 + 24x_1^4 x_4 + 84x_1^4 x_2^2 + 96x_1^2 x_2 x_3 \\
- 48x_1 x_2^2 x_3 &- 96x_1 x_3 x_4 - 72x_2^2 x_4 - 72x_2^2 x_6 - 18x_4^2 \end{align*} \) |
| \([4][2^2] \otimes [S_2 [S_4]] \) | \( \begin{align*} 4x_1^8 &+ 24x_1^6 x_2 + 16x_1^5 x_3 + 24x_1^4 x_4 + 24x_1^4 x_2^2 \\
+ 72x_1^2 x_3 &- 96x_1^2 x_2 x_3 - 128x_1^2 x_2 x_4 + 48x_1 x_3 x_4 + 96x_1 x_3 x_4 \\
+ 72x_2^2 x_4 &+ 36x_2^4 \end{align*} \) |
| \([4][2^1] \otimes [S_2 [S_4]] \) | \( \begin{align*} 6x_1^8 &+ 24x_1^6 x_2 + 48x_1^5 x_3 - 60x_1^4 x_2^2 + 48x_1^4 x_4 - 72x_1^2 x_2^3 \\
- 96x_1^3 x_2 x_3 &+ 48x_1^2 x_2 x_3 + 96x_1 x_3 x_4 + 72x_1 x_3 x_4 - 18x_4^2 \end{align*} \) |
| \([4][1^9] \otimes [S_2 [S_4]] \) | \( \begin{align*} 2x_1^8 &+ 32x_1^5 x_3 - 60x_1^4 x_2^2 - 144x_1^2 x_2 x_4 + 128x_1^2 x_2^3 \\
+ 96x_1 x_2^2 x_3 &- 72x_4^2 + 18x_2^4 \end{align*} \) |
| \([31][31] \otimes [2]^{12} \) | \( \begin{align*} 9x_1^8 &+ 36x_1^6 x_2 - 36x_1^4 x_4 + 18x_1^4 x_2^2 - 36x_1^2 x_2^2 - 72x_1^2 x_2 x_4 \\
- 144x_8 &- 36x_4^2 + 180x_2^2 x_4 + 81x_4^2 \end{align*} \) |
| \([31][31] \otimes [12]^{12} \) | \( \begin{align*} 9x_1^8 &+ 36x_1^6 x_2 - 36x_1^4 x_4 + 18x_1^4 x_2^2 - 36x_1^2 x_2^2 - 72x_1^2 x_2 x_4 \\
+ 144x_8 &+ 108x_4^2 - 108x_2^2 x_4 - 63x_4^2 \end{align*} \) |
| \([31][2^2] \otimes [S_2 [S_4]] \) | \( \begin{align*} 12x_1^8 &+ 24x_1^6 x_2 - 48x_1^5 x_3 - 24x_1^4 x_4 + 24x_1^4 x_2^2 + 72x_1^2 x_2^3 \\
- 96x_1^3 x_2 x_3 &+ 48x_1^2 x_2 x_3 + 96x_1 x_3 x_4 - 72x_2^2 x_4 - 18x_4^2 \end{align*} \) |
<p>| ([31][2^1] \otimes [S_2 [S_4]] ) | ( \begin{align*} 18x_1^8 &amp;- 108x_4^2 x_2^2 + 144x_1 x_2^4 x_4 - 72x_2^2 + 18x_2^4 \end{align*} ) |
| ([31][1^9] \otimes [S_2 [S_4]] ) | ( \begin{align*} 6x_1^8 &amp;- 24x_1^6 x_2 + 48x_1^5 x_3 - 60x_1^4 x_2^2 + 72x_1^2 x_2 x_4 - 18x_2^4 \end{align*} ) |</p>
<table>
<thead>
<tr>
<th>$\Gamma$</th>
<th>$1152 \Gamma^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$[(2^2)[2^2]] \odot [2^1]$</td>
<td>$4x_1^8 - 32x_1^6x_2 + 24x_1^4x_2^2 + 64x_1^2x_3^2 - 96x_1x_2x_3^2 + 144x_4^2$</td>
</tr>
<tr>
<td></td>
<td>$- 192x_2x_6 + 84x_4^2$</td>
</tr>
<tr>
<td>$[(2^2)[2^2]] \odot [1^2]$</td>
<td>$4x_1^8 - 32x_1^6x_2 + 24x_1^4x_2^2 + 64x_1^2x_3^2 - 96x_1x_2x_3^2 + 144x_4^2$</td>
</tr>
<tr>
<td></td>
<td>$+ 192x_2x_6 - 12x_4^2$</td>
</tr>
<tr>
<td>$[(2^2)[2^1]] + S_2 [S_4]$</td>
<td>$12x_1^3 - 24x_1^5x_2 - 48x_1^5x_3 + 24x_1^4x_4 + 36x_1^2x_2^2 - 72x_1x_2x_3$</td>
</tr>
<tr>
<td></td>
<td>$+ 96x_1^3x_2x_3 + 48x_1x_2^2x_3 - 96x_1x_3x_4 + 72x_2^2x_4 - 36x_4^2$</td>
</tr>
<tr>
<td>$[(2^2)[1^4]] + S_2 [S_4]$</td>
<td>$4x_1^8 - 24x_1^6x_2 + 16x_1^4x_3 - 24x_1^4x_4 + 24x_1^2x_2^2 - 72x_1x_2x_3$</td>
</tr>
<tr>
<td></td>
<td>$+ 96x_1^3x_2x_3 - 128x_1^2x_3^2 + 48x_1x_2x_3^2 + 96x_1x_3x_4 - 72x_2^2x_4$</td>
</tr>
<tr>
<td></td>
<td>$+ 36x_4^2$</td>
</tr>
<tr>
<td>$[(2^2)[2^2]] \odot [2^1]$</td>
<td>$9x_1^8 - 36x_1^6x_2 + 36x_1^4x_4 + 18x_1^4x_2^2 + 36x_1^2x_3^2$</td>
</tr>
<tr>
<td></td>
<td>$- 72x_1^2x_2x_4^2 + 144x_2^2 - 36x_4^2$</td>
</tr>
<tr>
<td></td>
<td>$- 180x_2^2x_4 + 81x_4^2$</td>
</tr>
<tr>
<td>$[(2^2)[2^1]] \odot [1^2]$</td>
<td>$9x_1^8 - 36x_1^6x_2 + 36x_1^4x_4 + 18x_1^4x_2^2 + 36x_1^2x_3^2$</td>
</tr>
<tr>
<td></td>
<td>$- 72x_1^2x_2x_4^2 - 144x_2^2 + 108x_2^2x_4 + 108x_2^2x_4 - 63x_4^2$</td>
</tr>
<tr>
<td>$[(2^2)[1^4]] + S_2 [S_4]$</td>
<td>$6x_1^8 - 48x_1^6x_2 + 48x_1^5x_3 - 24x_1^4x_4 + 84x_1^4x_2^2 - 96x_1^3x_2x_3$</td>
</tr>
<tr>
<td></td>
<td>$- 48x_1^3x_2x_3 + 96x_1x_2x_3^2 - 72x_4^2 + 72x_2^2x_4 - 18x_4^2$</td>
</tr>
<tr>
<td>$[(1^8)[1^4]] \odot [2^1]$</td>
<td>$x_1^8 - 12x_1^5x_2 + 16x_1^5x_3 - 12x_1^4x_4 + 42x_1^4x_2^2 - 36x_1^2x_2^3$</td>
</tr>
<tr>
<td></td>
<td>$- 96x_1^3x_2x_3 + 72x_1^2x_2x_4^2 + 54x_1^2x_3^2 + 48x_1x_2x_3^2 - 96x_1x_3x_4$</td>
</tr>
<tr>
<td></td>
<td>$- 144x_2^2 + 108x_2^2x_4 - 180x_2^2x_4 + 192x_2x_4 + 33x_4^2$</td>
</tr>
<tr>
<td>$[(1^8)[1^4]] \odot [1^2]$</td>
<td>$x_1^8 - 12x_1^5x_2 + 16x_1^5x_3 - 12x_1^4x_4 + 42x_1^4x_2^2 - 36x_1^2x_2^3$</td>
</tr>
<tr>
<td></td>
<td>$- 96x_1^3x_2x_3 + 72x_1^2x_2x_4^2 + 54x_1^2x_3^2 + 48x_1x_2x_3^2 - 96x_1x_3x_4$</td>
</tr>
<tr>
<td></td>
<td>$+ 144x_2^2 - 36x_4^2 + 108x_2^2x_4 - 192x_2x_6 - 15x_4^2$</td>
</tr>
</tbody>
</table>

From Table VI, we obtain

$$Z^{[4]}_{11} = \frac{1}{24}(x_1^4 + 6x_1^2x_2 + 8x_1x_3 + 6x_4 + 3x_2^3),$$

$$Z^{[31]}_{11} = \frac{1}{24}(3x_1^4 + 6x_1^2x_2 - 6x_4 - 3x_2^3).$$
Table VIII. Character table of $S_2[S_4]$ obtained from the GCCI's in Table VII and the methods in Ref. 2.

| $S_2[S_4]$ | 
| --- | --- |
| **Order** | **E** (1) | (12) | (13) | (14) | (123) | (124) | (134) | (1234) | (1243) | (1324) | (1342) | (123456) | (123457) | (123458) | (123459) |
| 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| 2 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| 3 | 6 | 4 | 3 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 |
| 4 | 4 | 2 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| 5 | 6 | 2 | 3 | 4 | 2 | -2 | -2 | -2 | -2 | -2 | -2 | -2 | -2 | -2 | -2 |
| 6 | 2 | 0 | 2 | 0 | 2 | -2 | -2 | 0 | -2 | 2 | 0 | 0 | 0 | 0 | -2 |
| 7 | 9 | 3 | 0 | -3 | -3 | 1 | -1 | 0 | -1 | 0 | 0 | 0 | 0 | -1 | 1 | 0 | 1 | 3 |
| 8 | 9 | 3 | 0 | -3 | -3 | 1 | -1 | 0 | -1 | 0 | 0 | 0 | 0 | -1 | 1 | 1 | 1 | 3 |
| 9 | 12 | 2 | -3 | -3 | 2 | 4 | 0 | 2 | -1 | 0 | 0 | 0 | 0 | -2 | 0 | 0 | 0 | 4 |
| 10 | 18 | 0 | 0 | 0 | -6 | -2 | 0 | 0 | 2 | 0 | 0 | 0 | 0 | -2 | 0 | 0 | 0 | 2 |
| 11 | 6 | -2 | 3 | -4 | 2 | -2 | -2 | 2 | 1 | 0 | -1 | -1 | 0 | 2 | 0 | 0 | 0 | -2 |
| 12 | 4 | 0 | -2 | 0 | 4 | 0 | 0 | 0 | 0 | 1 | -2 | 0 | 0 | 0 | -2 | 0 | 0 | 4 |
| 13 | 4 | 0 | -2 | 0 | 4 | 0 | 0 | 0 | 0 | 1 | -2 | 0 | 0 | 0 | -2 | 0 | 0 | 4 |
| 14 | 12 | -2 | -3 | -2 | 4 | 0 | -2 | 1 | 0 | 0 | -1 | 0 | 0 | 0 | 2 | 0 | 0 | -4 |
| 15 | 14 | 0 | -2 | 1 | -2 | -4 | 0 | 2 | -1 | 1 | 0 | 0 | 0 | -2 | 0 | 0 | 0 | 4 |
| 16 | 16 | 9 | 0 | 3 | -3 | 3 | 1 | 0 | -1 | 0 | 0 | 0 | 0 | 1 | 1 | 1 | 1 |
| 17 | 9 | 0 | 0 | 0 | 3 | -3 | 3 | 1 | 0 | -1 | 0 | 0 | 0 | 0 | 1 | 1 | 1 |
| 18 | 12 | 6 | -4 | 5 | -2 | 2 | 2 | 0 | -1 | 0 | 0 | 0 | -1 | 1 | 0 | 2 | 0 | 0 | -2 |
| 19 | 12 | 1 | -1 | 1 | -1 | 1 | 1 | -1 | 1 | 1 | 1 | -1 | 1 | 1 | -1 | 1 | 1 | 1 |
| 20 | 12 | 1 | -1 | 1 | -1 | 1 | 1 | -1 | 1 | 1 | 1 | -1 | 1 | 1 | -1 | 1 | 1 | 1 |

Therefore, for $\Gamma_3 = [4][31] \uparrow S_2[S_4]$, $P^{\Gamma_3}$ is

$$P^{\Gamma_3} = \frac{3}{24}(x_1^2 + 6x_1^2x_2 + 8x_1^2x_3 + 6x_4 + 3x_3^2) \cdot \frac{3}{24}(3x_1^4 + 6x_1^2x_2 - 6x_4 - 3x_3^2)$$

$$= \frac{3}{72}(3x_1^8 + 24x_1^6x_2 + 24x_1^5x_3 + 12x_1^4x_4 + 42x_1^2x_2^2 + 48x_1^3x_2x_3$$

$$- 24x_1x_2^2x_3 - 48x_1x_3x_4 - 36x_4^2 - 36x_2^2x_4 - 9x_2^2).$$

Hence $1152P^{\Gamma_3}$ is the expression shown in Table VII. From this expression the character corresponding to all the conjugacy classes can be immediately determined except the conjugacy classes with the cycle types $x_1^2x_2^2$, $x_1^2$, $x_2^2x_3$, and $x_2^3$. For example, the character corresponding the conjugacy class (12) is $\frac{1}{12}$ times
the coefficient of $x_1^4x_2$ in $1152P^3$. The multiplication factor is $\frac{1}{12}$ because the order of this conjugacy class is 12. Thus, this character is $\frac{4}{12} = 4$. The character corresponding to the conjugacy classes with the cycle types $x_1^4x_2^2$, etc., can be determined if the character of one of the conjugacy classes of the same cycle type is known.

5. Generalized Isomer Enumerations

One of the interesting chemical applications of combinatorics is the enumeration of chemical isomers which are equivalence classes of maps from the set of vertices of a chemical graph to chemical substituents. Several papers [11–12, 21–48] have appeared in both mathematical and chemical literature ever since the appearance of the paper of Pólya [48]. Here we consider an important generalization using the formalism in Section 2.

The complete interconversions obtainable by the allowed symmetry operations are best described by the irreducible representations contained in each equivalence class formed by isomers. Each isomer or a pattern (in Pólya terminology) is a representative of the set of functions that are transformable into one another by the action of the molecular symmetry group. The set of functions in any equivalence class transforms as a reducible representation and it will be interesting to know the irreducible representations contained in each pattern. The GCCI's introduced in earlier sections with Pólya substitution are the generators of irreducible representations contained in patterns. The coefficient of a typical term $w^b_1w^{b_2}_2\cdots$ in the GCCI corresponding to the irreducible representation $\Gamma$ generates the frequency of occurrence of $\Gamma$ in the set of functions with the weight $w^b_1w^{b_2}_2\cdots$.

Let us illustrate the above method with generalized isomer enumeration of nonrigid hydrazine molecule. Replace the protons of this molecule by the substituents $a$ and $b$ so that the chemical formula is $N_2a_2b_2$. The rotational subgroup of the nonrigid molecule is described by the wreath product $S_2[S_2]$ [1]. The GCCI's of the various irreducible representations of $S_2[S_2]$ with labels in accordance to chemical literature are in Table IX. If we replace each $x_k$ by $\Sigma(w(r))^k$, we obtain generators of generalized isomer enumerations. Such generators are

\[ GF^{A_1} = P^{A_1}_G(x_k \to a^k + b^k) = a^4 + a^3b + 2a^2b^2 + ab^3 + b^4, \]
\[ GF^{B_1} = P^{B_1}_G(x_k \to a^k + b^k) = a^3b + a^2b^2 + ab^3, \]
\[ GF^{E} = P^{E}_G(x_k \to a^k + b^k) = a^3b + a^2b^2 + ab^3, \]
\[ GF^{B_2} = P^{B_2}_G(x_k \to a^k + b^k) = a^2b^2, \]
\[ GF^{A_2} = P^{A_2}_G(x_k \to a^k + b^k) = 0. \]

The coefficient of $a^2b^2$ in the generator corresponding to an irreducible representation $\Gamma$ gives the number of times $\Gamma$ occurs in the set of functions with the weight $a^2b^2$. The generator corresponding to the totally symmetric rep-
TABLE IX. GCCI's of the group $S_3[S_2]$.

<table>
<thead>
<tr>
<th>$r$</th>
<th>$8P^X_G$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1$</td>
<td>$x_1^4 + 2x_1^2x_2 + 3x_2^2 + 2x_4$</td>
</tr>
<tr>
<td>$A_2$</td>
<td>$x_1^4 - 2x_1^2x_2 - x_2^2 + 2x_4$</td>
</tr>
<tr>
<td>$B_1$</td>
<td>$x_1^4 + 2x_1^2x_2 - x_2^2 - 2x_4$</td>
</tr>
<tr>
<td>$B_2$</td>
<td>$x_1^4 - 2x_1^2x_2 + 3x_2^2 - 2x_4$</td>
</tr>
<tr>
<td>$E$</td>
<td>$2x_1^4 - 2x_2^2$</td>
</tr>
</tbody>
</table>

TABLE X. Generalized isomer enumeration of substituted hydrazine. The set of functions from the set of vertices to substituents with the weight $a^2b^2$, the patterns (isomers), and the irreducible representations contained in each pattern are shown.

<table>
<thead>
<tr>
<th>Functions</th>
<th>Pattern</th>
<th>Irreducible Representations</th>
</tr>
</thead>
<tbody>
<tr>
<td>$aa$ $bb$</td>
<td>$bb$ $aa$</td>
<td>$A_1 \otimes B_1$</td>
</tr>
<tr>
<td>$ab$ $ab$</td>
<td>$ab$ $ba$</td>
<td>$A_1 \otimes B_2 \otimes E$</td>
</tr>
<tr>
<td>$ba$ $ab$</td>
<td>$ba$ $ba$</td>
<td></td>
</tr>
</tbody>
</table>

representation is the generator of patterns. Thus the coefficient of $a^2b^2$ in the $A_1$ generator shows that there are two isomers (patterns) for this molecule. The two functions corresponding to the isomer I (in Table X) transform as $A_1 \oplus B_1$ as generated by GCCI's. The functions which are in the equivalence class formed by the isomer II transform as $A_1 \oplus E \oplus B_2$. Equivalently, the symmetry operations of this molecule transform the maps from four vertices of the hydrazine to substituents $a$ and $b$ with the weight $a^2b^2$ into two equivalence classes. Each class splits into direct sum of irreducible representations $A_1 \oplus B_1$ and $A_1 \oplus B_2 \oplus E$, respectively. Further applications to isomerization reactions can be found in Ref. 51.

Acknowledgments

The author thanks Professor Kenneth S. Pitzer for his encouragement. This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Chemical Sciences Division of the U.S. Department of Energy under Contract No. W-7405-ENG-48.
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Received March 18, 1982
Accepted for publication May 17, 1982